

Methanesulfonic acid
75-75-2 | DTXSID4026422

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: 7.23 °C

Global applicability domain: Inside

Local applicability domain index: 6.10e-01

Confidence level: 6.07e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Methanesulfonic acid</div> <div>Measured: 20.0</div> <div>Predicted: 7.23</div>	<div>Image not found</div> <div>Ethanesulfonic acid</div> <div>Measured: -17.0</div> <div>Predicted: -11.4</div>	<div>Image not found</div> <div>1-Propanesulfonic acid</div> <div>Measured: 7.50</div> <div>Predicted: -6.73</div>
<div>Image not found</div> <div>Propane-2-sulphonic acid</div> <div>Measured: -37.0</div> <div>Predicted: -8.58</div>	<div>Image not found</div> <div>1-Butanesulfonic acid</div> <div>Measured: -15.2</div> <div>Predicted: 3.49</div>	